

Modeling the Transient Effects during the Hot-Compression of Wood-Based Composites

by

Balazs G. Zombori

Frederick A. Kamke, Chairman

(Abstract)

A numerical model based on fundamental engineering principles was developed and validated to establish a relationship between process parameters and the final properties of wood-based composite boards. The model simulates the mat formation, then compresses the reconstituted mat to its final thickness in a virtual press. The number of interacting variables during the hot-compression process is prohibitively large to assess a wide variety of data by experimental means. Therefore, the main advantage of the model based approach that the effect of the hot-compression parameters on the final properties of wood-based composite boards can be monitored without extensive experimentation.

The mat formation part of the model is based on the Monte Carlo simulation technique to reproduce the spatial structure of the mat. The dimensions and the density of each flake are considered as random variables in the model, which follow certain probability density distributions. The parameters of these distributions are derived from data collected on industrial flakes by using an image analysis technique. The model can simulate the structure of a three-layer oriented strandboard (OSB) mat as well as the structure of random fiber networks. A grid is superimposed on the simulated mat and the number of flakes, the thickness, and the density of the mat at each grid point are computed. Additionally, the model predicts the change in several void volume fractions within the mat and the contact area between the flakes during consolidation. The void volume fractions are directly related to the physical properties of the mat, such as thermal conductivity, diffusivity, and permeability, and the contact area is an indicator of the effectively bonded area within the mat.

The heat and mass transfer part of the model predicts the change of air content, moisture content, and temperature at designated mesh points in the cross section of the mat during the hot-compression. The water content is subdivided into vapor and bound water components. The free water component is not considered in the model due to the low (typically 6-7 %) initial moisture content of the flakes. The gas phase (air and vapor) moves by bulk flow and diffusion, while the

bound water only moves by diffusion across the mat. The heat flow occurs by conduction and convection. The spatial derivatives of the resulting coupled partial differential equations are discretized by finite differences. The resulting ordinary differential equation in time is solved by a differential-algebraic system solver (DDASSL). The internal environment within the mat can be predicted among different initial and boundary conditions by this part of the hot-compression model.

In the next phase of the research, the viscoelastic (time, temperature, and moisture dependent) response of the flakes was modeled using the time-temperature-moisture superposition principle of polymers. A master curve was created from data available in the literature, which describes the changing relaxation modulus of the flakes as a function of moisture and temperature at different locations in the mat. Then the flake mat was compressed in a virtual press. The stress-strain response is highly nonlinear due to the cellular structure of the mat. Hooke's Law was modified with a nonlinear strain function to account for the behavior of the flake mat in transverse compression. This part of the model gives insight into the vertical density profile formation through the thickness of the mat.

Laboratory boards were produced to validate the model. A split-plot experimental design, with three different initial mat moisture contents (5, 8.5, 12 %), three final densities (609, 641, 673 kg/m³ or 38, 40, 42 lb/ft³), two press platen temperatures (150, 200 °C), and three different press closing times (40, 60, 80 s) was applied to investigate the effect of production parameters on the internal mat conditions and the formation of the vertical density profile. The temperature and gas pressure at six locations in the mat, and the resultant density profiles of the laboratory boards, were measured. Adequate agreement was found between the model predicted and the experimentally measured temperature, pressure, and vertical density profiles.

The complete model uses pressing parameters (press platen temperature, press schedule) and mat properties (flake dimensions and orientation, density distribution, initial moisture content and temperature) to predict the resulting internal conditions and vertical density profile formation within the compressed board. The density profile is related to all the relevant mechanical properties (bending strength, modulus of elasticity, internal bond strength) of the final board. The model can assist in the optimization of the parameters for hot-pressing wood-based composites and improve the performance of the final panel.

Acknowledgements

I wish to express my sincere gratitude to my major advisor Dr. Frederick A. Kamke, who directed me towards the challenging field of wood-based composites, and whose office door was always open for discussion. I owe many thanks to Dr. Layne T. Watson who helped me through the difficulties of code writing and debugging. Appreciation is also extended to my committee members Dr. J. Daniel Dolan, Dr. Charles E. Frazier, Dr. Elemer M. Lang, and Dr. Joseph R. Loferski for their valuable input, and ongoing support during the project.

The staff of the Brooks Forest Products Center made daunting tasks easy, therefore special thanks to Kenneth L. Albert, Robert S. Carner, Carlisle Price, and Harrison Sizemore, for helping me to install the measuring system, and Sharon C. Daley, and Angie G. Riegel for the morning coffees, and for smoothing my administration difficulties.

Finally, I owe tremendous appreciation to my family. They gave me the drive and freedom to be independent and made me believe that I am capable to undertake this endeavour.

This research was funded by the USDA National Research Initiative Competitive Grant Program (IRS No. 54-6001805). The financial support is greatly appreciated.

Table of Contents

Chapter 1. Project Description...1	
1.1 Introduction...1	
1.2 General Structure of Hot-Compression Model...2	
1.3 Technical Objective...4	
1.4 Rationale and Significance...4	
1.5 Structure of Dissertation...6	
References...7	
Chapter 2. Simulation of the Mat Formation Process...8	
Summary...8	
2.1 Introduction...9	
2.2 Background...10	
2.3 Model Development...12	
2.3.1 General Model Development...12	
2.3.2 Monitoring Structural Changes of the Mat during Compression...18	
2.4 Materials and Methods...20	
2.4.1 Database Assessment for Input Values of the Model...20	
2.4.2 Experimental Validation of the Model...22	
2.5 Results and Discussion...22	
2.5.1 General Characteristics and Probability Density Functions of the Input Variables...22	
2.5.2 General Validation of the Model...28	
2.5.3 Simulation of a Three-Layer Oriented Strand Board Mat...31	
2.5.4 Simulation of a Random Fiber Network...37	
2.6 Conclusions...37	
References...39	
Chapter 3. Modeling the Heat and Mass Transfer Phenomena during the Hot-Compression of Wood-Based Composites...41	
Summary...41	
3.1 Introduction...42	
3.2 Background...43	
3.3 Model Development...46	
3.3.1 Assumptions...46	
3.3.2 Governing Equations...47	
3.3.3 Transport Mechanisms...49	

3.3.4 Sorption Isotherms...	54
3.3.5 Physical and Transport Properties...	54
3.3.6 Thermodynamic Relationships...	63
3.3.7 Partial Pressures...	65
3.3.8 Initial and Boundary Conditions...	66
3.4 Numerical Solution...	69
3.4.1 Discretization at the Internal Points...	69
3.4.2 Discretization at the Boundary Points...	75
3.4.3 Solution of the ODE-Algebraic Equation System...	76
3.5 Results of a Simulation Run...	79
3.5.1 The Dynamic Nature of Hot Compression...	79
3.5.2 Detailed Analysis...	87
3.6 Conclusions...	101
Nomenclature...	102
References...	105
Chapter 4. Validation and Sensitivity Study of the Heat and Mass Transfer Model...	109
Summary...	109
4.1 Introduction...	110
4.2 Background...	112
4.3 Materials and Methods...	115
4.3.1 Panel Manufacture...	115
4.3.2 Temperature and Total Pressure Measurement...	119
4.3.3 Hot-Compression Simulation Runs...	120
4.4 Comparison of the Experimental and Model Predicted Internal Environment...	121
4.5 Effect of Hot-Pressing Parameters on the Internal Mat Environment...	125
4.6 Sensitivity Study of the Model...	131
4.7 Conclusions...	139
References...	140
Chapter 5. Modeling the Transverse Compression of Wood-Based Composites...	143
Summary...	143
5.1 Introduction...	144
5.2 Background...	145
5.3 Model Development...	147
5.3.1 Nonlinear Transverse Compression Behavior of the Flakes...	147
5.3.2 Viscoelastic Behavior of the Flakes...	152

5.3.3 Nonlinear Viscoelastic Behavior of the Mat in Transverse Compression...	164
5.4 Results of a Simulation Run...	174
5.5 Conclusions...	177
Nomenclature...	178
References...	179
Chapter 6. Validation of the Transverse Compression Model...	182
Summary...	182
6.1 Introduction...	182
6.2 Background...	183
6.3 Materials and Methods...	188
6.3.1 In situ Measurement of Mat Density...	188
6.3.2 Measurement of the Final Density Profile...	191
6.4 Results and Discussion...	192
6.4.1 In-situ Density Measurements...	192
6.4.2 Final Density Profiles...	197
6.5 Conclusions...	199
References...	200
Chapter 7. Final Conclusions and Recommendations...	203
7.1 Final Conclusions...	203
7.2 Recommendations...	204
Appendix A...	206

List of Tables

Table 2.1.	Descriptive statistics of core and face layer flake properties....23
Table 2.2.	Results of the goodness-of-fit tests. The tests were performed with a 95% confidence level....24
Table 2.3.	Descriptive statistics of experimental and simulated board horizontal densities....29
Table 2.4.	Parameters of the fitted Weibull distributions....30
Table 3.1.	Hot compression parameters used in the simulation....80
Table 4.1.	Split-plot experimental design for panel manufacture....115
Table 4.2.	Manufacturing specifications and out-of-press moisture contents and densities of the boards....117
Table 4.3.	The relative position of the internal temperature and gas pressure probes measured from probe location 6....118
Table 4.4.	The base and perturbed value of the model parameters for the sensitivity study....132
Table 5.1.	Parameters for the regression equations describing the temperature shift factor $\log a(T)$ as a function of temperature for different moisture contents....160
Table 5.2.	Moisture shift factor $\log a(M)$160
Table 5.3.	Parameters for the Maxwell elements fit to the relaxation modulus master curve....162
Table 5.4.	The compression parameters used in the simulation....174
Table 6.1.	Experimental design for the gamma-ray density measurements....190

List of Figures

- Figure 2.1. Flow diagram of the mat reconstruction routine....13
- Figure 2.2. Flow diagram of the mat property calculations....14
- Figure 2.3. Decision rule of the "triangulation" algorithm....15
- Figure 2.4. Decision rule of the "left" algorithm....16
- Figure 2.5. Flow diagram of the press closing simulation....17
- Figure 2.6. Typical digital image of face layer strands captured by the image analysis system....20
- Figure 2.7. Frequency histogram of core and face layer strand width. The fitted three-parameter gamma distribution is overlaid....25
- Figure 2.8. Frequency histogram of core and face layer strand thickness. The fitted three-parameter gamma distribution is overlaid....25
- Figure 2.9. Frequency histogram of core and face layer strand density. The fitted three-parameter gamma distribution is overlaid....26
- Figure 2.10. Frequency histogram of core and face layer strand length....26
- Figure 2.11. Calculated area and perimeter (face) versus measured area and perimeter distributions....27
- Figure 2.12. Density histograms generated from the experimental and predicted horizontal density data....28
- Figure 2.13. The reconstructed three-layer OSB mat. The mat area is 450 x 450 mm....32
- Figure 2.14. Contour map of the number (a.) and the total thickness (b.) of strands at the grid points....33
- Figure 2.15. Predicted horizontal density distribution of the compressed mat....34
- Figure 2.16. Simulated contact area and void volume as a function of mat compression strain....35
- Figure 2.17. Simulated mat and flake density as a function of mat compression strain....36
- Figure 2.18. The simulation results of the deposition of 400 fibers on a 7 x 7 mm area. The orientation of the fibers is unrestricted....38
- Figure 3.1. The effect of orientation angle and degree of alignment on the thermal conductivity of the flakes at the in-plane direction of the mat....57
- Figure 3.2. The parallel and series arrangement of the flakes and air in the out-of-plane and in-plane mat directions....58
- Figure 3.3. The effect of flake density and moisture content on the thermal conductivity of the mat in the out-of-plane and in-plane direction....59
- Figure 3.4. The effect of the elimination of the space among the flakes during compaction on the thermal conductivity of the mat....59

- Figure 3.5. Permeability as a function of mat density at the out-of-plane and in-plane directions....61
- Figure 3.6. The effect of the elimination of the void during compaction on the diffusivity of the mat....62
- Figure 3.7. Interpretation of the initial and boundary conditions....66
- Figure 3.8a. Finite difference mesh in one dimension....70
- Figure 3.8b. The finite difference mesh superimposed on the vertical midplane of the board....73
- Figure 3.9a. Flow diagram of the hot compression module....77
- Figure 3.9b. Flow diagram of the right hand side routine....78
- Figure 3.10. Predicted temperature and moisture profiles during the hot compression of a single-layer strandboard....81
- Figure 3.11. Predicted total pressure and relative humidity profiles during the hot compression of a single-layer strandboard....82
- Figure 3.12. Predicted air and vapor partial pressure profiles during the hot compression of a single-layer strandboard....83
- Figure 3.13. Predicted adhesive cure index profiles during the hot compression of a single-layer strandboard....84
- Figure 3.14. The vertical midplane of the board where the model predicted results are calculated....87
- Figure 3.15. Evolution of temperature (a.), moisture content (b.), total pressure (c.), and relative humidity (d.) in the vertical midplane of the board with time for several positions in the vertical direction....89
- Figure 3.16. Evolution of temperature (a.), moisture content (b.), total pressure (d.), and relative humidity (d.), in the vertical midplane of the board with time for several positions in the horizontal direction....90
- Figure 3.17. Evolution of air (a., b.) and vapor (c., d.) partial pressures in the vertical midplane of the board with time for several positions in the vertical (left) and horizontal (right) directions....91
- Figure 3.18. Vertical profiles of temperature (a.), moisture content (b.), total pressure (c.), and relative humidity (d.) in the vertical midplane of the board for different times during the press schedule varying form 10 s to 480 s....97
- Figure 3.19. Horizontal profiles of temperature (a.), moisture content (b.), total pressure (c.), and relative humidity (d.), in the vertical midplane of the board for different times during the press schedule varying form 10 s to 480 s....98
- Figure 3.20. Vertical (left) and horizontal (right) profiles of air (a., b.) and vapor (c., d.) partial pressures in the vertical midplane of the board for different times during the press schedule varying form 10 s to 480 s....99

- Figure 4.1. The intended locations of the six thermocouples and pressure probes in the vertical midplane of the mat....116
- Figure 4.2. The laboratory hot-press together with the six temperature and pressure probes....120
- Figure 4.3. Plot of temperature at the six measuring locations as a function of press time at 150 °C platen temperature....122
- Figure 4.4. Plot of gauge total pressure at the six measuring locations as a function of press time at 150 °C platen temperature....122
- Figure 4.5. Plot of temperature at the six measuring locations as a function of press time at 200 °C platen temperature....123
- Figure 4.6. Plot of gauge total pressure at the six measuring locations as a function press time at 200 °C platen temperature....123
- Figure 4.7. The effect of different mat characteristics and press schedules on the temperature at the core of the mat (probe location 6)....126
- Figure 4.8. The effect of different mat characteristics and press schedules on the gauge total pressure at the core of the mat (probe location 6)....127
- Figure 4.9. The effect of different mat characteristics and press schedules on the average moisture content of the mat (probe locations 6)....128
- Figure 4.10. The sensitivity coefficients of core temperature (a.), total gas pressure (b.), and average moisture content with time as a function of the transport properties of the mat....134
- Figure 4.11. The sensitivity coefficients of core temperature (a.), total gas pressure (b.), and average moisture content with time as a function of the transport properties of the boundary at the face of the mat....136
- Figure 4.12. The sensitivity coefficients of core temperature (a.), total gas pressure (b.), and average moisture content with time as a function of the transport properties of boundary at the edge of the mat....137
-
- Figure 5.1. Characteristic stress-strain diagram for cellular materials....147
- Figure 5.2. The nonlinear strain function as a function of relative density....149
- Figure 5.3. The barrelling effect....150
- Figure 5.4. The nonlinear strain function as a function of expansion ratio....151
- Figure 5.5. Typical change of the relaxation modulus of an amorphous polymer with time and temperature....152
- Figure 5.6. Diluent dependence of T_g of lignin and hemicellulose as described by the Kwei model....154
- Figure 5.7. Linear viscoelastic models: Kelvin chain and Maxwell ladder....158
- Figure 5.8. Relaxation modulus master curve plotted against reduced time....159

- Figure 5.9. The temperature and moisture content shift factor. The second order surface was fit to data derived by Wolcott (1989)....161
- Figure 5.10. The fitted relaxation modulus as function of reduced time....163
- Figure 5.11. Representation of the compression of the strand columns....164
- Figure 5.12. Representation of the compression behavior of a flake column by a series of Maxwell ladders....167
- Figure 5.13. Representation of the compression behavior of a flake column by a series of springs....171
- Figure 5.15. The evolution of the vertical density profile with time....175
- Figure 5.16. The vertical density profile at selected times during the hot compression....175
- Figure 5.17. The five stages of vertical density profile formation during hot pressing....176
-
- Figure 6.1. The position of the gamma ray sources....188
- Figure 6.2. The QMS x-ray density profiler....191
- Figure 6.3. The effect of panel final density on the evolution of density at 50 % and 25 % locations in the mat during the press schedule....193
- Figure 6.4. The effect of platen temperature on the evolution of density at 50 % and 25 % locations in the mat during the press schedule....194
- Figure 6.5. The effect of press closing time on the evolution of density at 50 % and 25 % locations in the mat during the press schedule....195
- Figure 6.6. The effect of different mat characteristics and press schedules on the final vertical density profile....198

List of Symbols

Constants

R = universal gas constant 8.31696 (J / mol / K)

M_a = molar weight of air 0.028968 (kg / mol)

M_v = molar weight of vapor 0.018016 (kg / mol)

ρ_{cw} = density of the cell wall 1500 (kg / m³)

Symbols

A = reaction constant

C = specific heat of wet wood (J / m³ / K)

C_p = heat capacity (J / kg / K)

D_{AB} = binary gas diffusivity for air – vapor mixture (m² / s)

D_{eff} = effective gas diffusivity (m² / s)

D_m = mat gas diffusivity (kg / m / s)

D_b = bound water diffusivity (kg s / m³)

$D(t)$ = Creep Compliance (1 / Pa)

$E(t)$ = Relaxation Modulus (Pa)

E = Young' s Modulus (Pa)

E_{cw} = Young' s Modulus of the cell wall (Pa)

E_i = modulus of the spring (Pa)

E = activation energy (J / mol)

F = extent of reaction (cure index)

G = heat generation (J / m³)

K_g = specific gas permeability of dry wood (m³ / m)

K_m = mat superficial gas permeability (s)

L = board dimension (m)

L_i = dimension of column (m)

M = moisture (%)

M_p = molar weight (kg / mol)

P = total pressure (Pa)

R = universal gas constant (J / mol / K)

S = entropy (J / mol / K)

T = temperature (K)

T_g = glass transition temperature (°C)

$a(T, M)$ = temperature and moisture shift factor

c_p = heat convection flux ($J/m^2/s$)

h_p = enthalpy (J/kg)

k = thermal conductivity

n_p = mass flux ($kg/m^2/s$)

n = order of reaction

p = partial pressure (Pa)

q = heat conduction flux ($J/m^2/s$)

t' = reduced time (s)

t = time (s)

α = attenuation factor for vapor diffusivity in the flakes

ϵ = strain

ϵ_y = yield strain of the cell wall (0.015 for wood)

Θ = rotation angle (deg)

ϕ_1, ϕ_2 = degree of alignment (deg)

η = viscosity ($kg/m/s$)

η_i = viscosity of the dashpot ($kg/m/s$)

λ = heat of vaporization (J/kg)

μ = expansion ratio

μ_p = chemical potential (J/kg)

ρ_a = density of air (kg/m^3)

ρ_b = density of bound water (kg/m^3)

ρ_d = density of dry wood (kg/m^3)

ρ_r = relative density

$\rho_r(\epsilon)$ = relative density function

ρ_v = density of vapor (kg/m^3)

σ = stress (Pa)

τ = retardation or relaxation time (s)

$\psi(\epsilon)$ = nonlinear strain function

ζ_{lf} = lumen fraction in the flakes

ζ_{sm} = space fraction in the mat

ζ_{vm} = void (space + lumen) fraction in the mat

ζ_{lm} = lumen fraction in the mat

\mathcal{H}^j = external heat transfer coefficient ($J/m^2/s/K$)

\mathcal{K}^j = external bulk flow coefficient (m)

\mathcal{D}^j = external diffusion coefficient (m/s)

Superscripts

B = boundary point

b = bottom boundary

edge = left and right boundary

face = top and bottom boundary

j = represents boundaries (top, bottom, left, right)

l = left boundary

r = right boundary

t = top boundary

∞ = environment

y = horizontal coordinate in the width of the board

z = vertical coordinate in the thickness of the board

Subscripts

E = east from the actual point

L = longitudinal anatomical direction in solid wood

N = north from the actual point

P = actual point

S = south from the actual point

T = transverse (radial and tangential) anatomical direction in solid wood

W = west from the actual point

a = air

b = bound water

cw = cell wall

d = dry wood

dp = dew point

e = east interface

f = flake

fsp = fiber saturation point

g = gas phase (air + vapor)

i = x direction

j = y direction

k = z direction

l = lumen (hole in the flake)

m = mat

n = north interface

p = phase (air, vapor, bound water)

s = space (hole in the mat)

s = south interface

sat = saturation

v = vapor

v = void (space + lumen)

w = water

w = west interface